Appendix G

Development of Screening Levels and Cleanup Levels for Polychlorinated Biphenyls (PCBs)

1.0 Introduction

As part of the development of a DEQ Strategy for addressing PCB contaminated sites, a subgroup was formed to evaluate the feasibility of developing statewide screening levels and cleanup levels for PCBs in soils and sediments. The purpose of the screening levels is to help prioritize sites or locations that would require further investigation or source assessment. The subgroup cautions against relying solely on sediment screening levels to prioritize sites. The screening levels are one of several elements to be considered in an overall prioritization strategy. Ideally, all locations with elevated fish tissue concentrations resulting in a consumption advisory would warrant further investigation. The screening levels would be a tool to prioritize those sites.

For soils, the subgroup identified published values that can be used for screening restricted and unrestricted use sites. These are described in Section 2.1.

For sediments, the initial focus of the subgroup was to identify or develop risk-based screening levels that would not result in fish tissue concentrations exceeding the Virginia Department of Health (VDH) screening level of 54 ug/kg (rounded to 50 ug/kg). The subgroup identified two methods for developing risk-based screening levels. These two approaches are discussed in Sections 2.2.1 and 2.2.2 below. However, the subgroup recognized that the risk-based screening levels would likely be too low to be an effective prioritization tool. The risk-based approaches confirmed that very low levels of PCBs (1.8 to 49 ppb) in sediments could result in elevated fish tissue concentrations. Therefore the subgroup also compiled data from previous monitoring locations and identified the levels corresponding to various percentiles of the data set. The purpose of compiling the percentile values was to identify a more practical level to insure that the worst locations would be addressed first. The percentile approach is presented in Section 3.

Cleanup levels would be applied to sites/locations for which it has been determined that remedial action is necessary. Because site-specific conditions vary widely throughout the state, the subgroup decided that it would not be appropriate to set statewide cleanup levels for sediments. The subgroup identified a tool that may be useful in developing site-specific cleanup levels. This tool, the Bioaccumulation and Aquatic System Simulator (BASS) model, is discussed in Section 4.1. Cleanup levels for soil should also be selected on a site-specific basis. However, for most sites, the soil cleanup levels identified in the Toxic Substances Control Act (TSCA) will be appropriate. These are presented in Section 4.2.

2.0 Risk-Based Screening Levels

2.1 Soil

Screening levels for soil are based on the EPA Region III Risk-based concentration (RBC) table (EPA, 2004a,b). They are based on a 10^{-6} cancer risk and standard default exposure factors. For residential or unrestricted-use sites the level is 0.32 mg/kg. For sites restricted to commercial/industrial use the screening level is 1.4 mg/kg. The equations and exposure factors used to derive these screening levels are presented in Appendix E.1.

2.2 Sediment

The subgroup was not able to identify any published screening levels for sediment based on bioaccumulation to the human food chain. However, two methods for calculating these levels were identified. Both the biota-sediment accumulation factor (BSAF) approach and the BASS model and their resulting screening levels are discussed in the following sections.

The relationships between sediment concentrations of PCBs and the resulting concentrations in fish tissue are influenced by several different factors. These include certain chemical properties of the PCB congeners such as the hydrophobicity (*Kows*) of the PCB congeners and the rate of chemical metabolism in the food chain. Other factors are properties of the ecosystem, which influence the sediment-fish relationship on a site-specific basis. These site-specific factors include the sediment/water disequibibrum, relative benthic/pelagic connectivity of the food web, the complexity of the wood web, the trophic level of the fish, ecosystem temperature, food availability, feeding patterns, seasonal and diurnal movements, organism growth rates, lipid contents and weights (Burkhard et.al., 2003). All these site-specific variables make predicting a relationship between sediment and fish-tissue concentrations of PCBs an imprecise exercise.

Two approaches of predicting a sediment concentration that should not result in fish contamination levels exceeding 54 ppb were evaluated by the committee, the BASS model and BSAF approaches. Both methods resulted in predicted "acceptable" sediment concentrations often varying by an order of magnitude. Because of this imprecision, predicted BSAFs or the use of the BASS model should not be used alone to calculate sediment clean up levels or used as a stand-alone indication of unacceptable contaminated sediment. However, used in conjunction with known fish contamination data from the waterbody, as well as other site-specific considerations, they may be useful in helping to identify sediments that have an increased potential for fish contamination. Both methods predicted "acceptable" sediment concentrations of PCBs to be between 1.8 to 49 parts per billion. This informs us that there is a potential for fish to be contaminated with PCBs at unacceptable levels in waterbodies where sediment concentrations of PCBs are in the low parts per billion ranges.

2.2.1 BSAF Approach

The subgroup identified literature values for BSAFs, which relate the concentration in sediment to the concentration in fish tissue. The BSAFs were then used to back calculate sediment concentrations below which fish tissue concentrations would not be expected to exceed the Virginia Department of Health (VDH) trigger level of 54 ppb.

The BSAF values and resulting sediment screening levels that the subgroup reviewed are presented in Appendix E.2. The exposure factors and equation used to derive the acceptable tissue concentration are also presented. The BSAF values ranged from 1.1 to 30. This resulted in screening levels ranging from 1.8 to 49 ppb.

There are many uncertainties relating to the derivation of the BSAFs. These uncertainties include the following:

- BSAF values relate the organic carbon-normalized contaminant concentration in the sediment to the lipid-normalized concentration in fish tissue. Any given screening level would only be applicable to sediments with similar organic carbon content and fish with similar lipid content.
- Concentrations in migratory fish may not be directly related to sediment concentrations in a given area.
- BSAFs may be different for different species. Only one of the BSAFs that the subgroup reviewed was for catfish. None were based on carp. Catfish and carp are among the fish that frequently exceed VDH screening levels.
- The subgroup reviewed BSAFs that were derived from total PCBs based on congener analysis. The specific congeners in the sediment will vary from site to site and may influence the BSAF.
- BSAF values may vary based on characteristics of the water bodies from which they were derived. Therefore the screening values may not be directly comparable to specific sites in Virginia.

2.2.2 BASS Model

The BASS modeling software uses sediment or water PCB concentrations to help predict what levels will end up in different species of fish. It considers modeling factors, either variables or constants, for different habitats and other environmental conditions. A more detailed description of BASS and its potential applications for DEQ is presented in Appendix E.3. The model can be used to back-calculate a sediment screening level using some default assumptions and the VDH fish tissue screening level. The development of the calculation is presented on pages 3-5 of Appendix E.3. An example of a calculation originally derived with an MS Excel spreadsheet can be found in Appendix E.4.

The sediment screening level resulting from this calculation is 15 ppb. Note, however, that there are many uncertainties regarding the screening calculation. These include

- equilibrium between sediment and water column PCB concentrations
- time varying vs. constant exposures
- treating PCBs as a single chemical (e.g., not addressing differences in congener K_{ow})
- the ecology and physiology of the target fish species (i.e., growth rates, dietary composition, lipid contents, mobility, etc.)

3.0 Percentile Based Screening Levels

The purpose of the percentile calculation method was to establish a statewide distribution of sediment PCB concentrations, from which a sediment PCB action based trigger value, could be selected.

3.1 Data Collection & Usability

As an initial step, the PCB Screening Level Subgroup requested that all available PCB data sets generated through special studies by the DEQ Regional Offices be submitted to Central Office for analysis. The larger data set from the years 1995-2002, generated by the statewide Fish Tissue and Sediment Collection, was also considered. Data sets were received from PRO (James River), VRO (Avtex- Shenandoah River), SCRO (Roanoke River), TRO (Elizabeth River), and WCRO (New River). PCB data sets from SWRO were also considered.

Once the disparate PCB data sets were attained, a decision had to be made on the appropriateness of compiling and analyzing all the available data as different PCB methods were utilized. Since the Fish Tissue and Sediment data set was by far the largest with over 700 records, it made most sense to adopt the VIMS congener analytical method. The resulting definition for "Total PCBs" was the sum of possible 209 congeners, which are targeted by the analytical method. Besides the primary data set, other data sets meeting the above criteria were the James and New River Special Studies. The SCRO, SWRO, TRO and VRO data sets were excluded as Total PCBs did not meet the above definition (<30 targeted congeners), while the VRO data set was based on summed Aroclors. Soil and sediment samples collected from within facility treatment trains were excluded from the analysis. Quality assurance samples identified as duplicates were also excluded.

3.2 Method & Results

The appropriate data sets were combined in an Excel spreadsheet format and analyzed with the Percentile Worksheet Function. For each scenario described below, summary statistics such as count (n), minimum and maximum values, and average were provided. The targeted percentiles included 99^{th}, 95^{th}, 90^{th}, 85^{th}, 80^{th} and the quartiles (75^{th}, 50^{th}, and 25^{th}). The five scenarios used in the evaluation were as follows:

- Combined data (VIMS) from the statewide Fish Tissue & Sediment Monitoring Program plus special studies on the New and James Rivers.
- VIMS data generated for the statewide Fish Tissue & Sediment Monitoring Program (excluding non-detects and 0.0s).
- VIMS data generated for PRO's James River special studies (1997-1998 & 2003)
- VIMS data generated for WCRO's New River PCB special study.
- VIMS data generated for the statewide Fish Tissue & Sediment Monitoring Program and includes non-detects (1/2 of value) and 0.0s.

With much collaboration, it was decided to use the percentiles calculated from the Fish Tissue & Sediment Monitoring Program with the inclusion of one-half of non-detected values plus those sites reported as 0.0. The results for all other scenarios considered in this evaluation can be found in Appendix E.5. The rationale for selecting this data set is it is most representative of the statewide distribution of sediment PCB concentrations and contains a reduced number of biased sample sites (Table 1) when compared to the special studies, thus yielding a more appropriate percentile distribution.

Table 1. VIMS data generated for the statewide Fish Tissue & Sediment Monitoring Program and includes non-detects (1/2 of value) and 0.0s.

Total PCB Conc. ppb	**Percentile**	**Summary Statistics**	**value**
1,611.6	99th	Count (n)	709
81.7	95th	Minimum (ppb)	0.00
40.1	90th	Maximum (ppb)	82,235.4
19.6	85th	Average (ppb)	162.6
13.2	80th		
7.9	75th		
2.2	50th		
0.4	25th		

4.0 Cleanup Levels

4.1 Sediment

The BASS model that was discussed above may also be useful in deriving site-specific cleanup levels for sediment. The equation that was used to derive a screening level in Appendix E.3 can be modified with site-specific information to develop more appropriate cleanup levels for different watersheds. A site-specific value can be used for the organic carbon content of the sediment. Bioaccumulation factors for the specific congeners detected and the fish species of concern could be used. K_{ow} values for specific congeners could also be used to modify the model for specific locations.

4.2 Soil

For determining cleanup levels, the DEQ Office of Remediation Programs (Federal Facilities, VRP, Superfund) generally uses the levels designated in the Toxic Substances Control Act (TSCA). The TSCA levels are:

- Less than 1 ppm for high occupancy areas with no conditions
- Less than 10 ppm for high occupancy areas with a cap
- Less than 25 ppm for low occupancy areas with no conditions
- Less than 100 ppm for low occupancy areas with a cap

TSCA defines high occupancy as greater than 16.8 hours per week. (EPA, 1998)

5.0 Conclusions and Recommendations

For soil, the subgroup recommends that the EPA Region 3 RBCs be incorporated into the Statewide PCB Strategy to prioritize sites for further assessment. These levels are widely used throughout the region. They have been used for many years by other offices within DEQ. They have been adopted by the Virginia Voluntary Remediation Program (VRP) to determine contaminants of potential concern for risk assessment.

Based on the uncertainties associated with a sediment risk-based approach and the reality of hitting or missing PCBs during sediment collection, the subgroup recommends both the risk-based value (15 ppb) and the 95th percentile value (82 ppb) of the DEQ data set be considered within the PCB prioritization matrix, as opposed to using stand-alone sediment screening values.

As discussed in a previous section, there are several inherent uncertainties in the BSAF approach and the BASS model. The subgroup also looked at the risk-based screening levels in comparison to the data that have been collected by DEQ, and have determined that the value predicted by the BASS model (15 ppb) falls within the 80th to 85th percentile range of those data. The subgroup believes that it may not be feasible to investigate all of the locations that exceed this level, but yet it is appropriate to include this approach within the prioritization scheme, albeit at a lower weighting.

The data collected in the DEQ Fish Tissue and Sediment Monitoring program and other studies demonstrate that there is often no direct correlation between sediment levels and fish tissue levels. The subgroup is aware of cases where there are high fish tissue levels and low sediment levels. In many of these cases, the lack of elevated sediment data may simply be due to not having enough samples. On the other hand, it may be that local conditions are such that very low levels of PCBs in sediments may be bioavailable. Therefore, in order to insure that the worst locations in the state are addressed first, the subgroup recommends that the 95th percentile (82 ppb) also be considered within the prioritization matrix but with a greater weighting than that given to the risk-based number.

The subgroup recommends that the cleanup levels cited in TSCA be used for soils in most cases. In some cases, however, levels derived from a site-specific risk assessment may be appropriate.

The subgroup recommends that DEQ continue to evaluate the BASS model as a tool to develop site-specific cleanup levels for sediment.

6.0 References:

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Appendix E.1

Residential

VALUES USED FOR TARGET SOIL CONCENTRATION CALCULATIONS

Medium:	Soil
Exposure Medium:	Soil
Receptor:	Resident
Exposure Route:	Ingestion
Receptor Age:	Lifetime (age-adjusted)

Target Soil Concentration:
CS=RLx IF x 1/CSF

Intake Factor Equation:
IF=AT x 1/EF x 1/IR x 1/CF

Parameter Code	Parameter Definition	Units	Default Value	Rationale/ Reference	User Defined Value	Rationale/ Reference
CS	Target Soil Concentration	mg/kg	3.20E-01	calculated		
RL	Target Risk Level		1.00E-06	EPA		
CSF	Carcinogenic Slope Factor for PCBs	1/mg/kg-day	2.00E+00	EPA		
IR	Soil Ingestion Rate	mg-yr/kg-day	114	EPA		
EF	Exposure Frequency	days/year	350	EPA		
CF	Conversion Factor	kg/mg	1.E-06	EPA		
AT	Averaging Time	days	25,550	EPA		
IF-C	Intake Factor (Cancer)	days	6.40E+05	calculated		

Commercial/Industrial

VALUES USED FOR TARGET SOIL CONCENTRATION CALCULATIONS

Medium:	Soil
Exposure Medium:	Soil
Receptor:	Commercial/Industrial
Exposure Route:	Ingestion
Receptor Age:	Adult

Target Soil Concentration:
CS=RLx IF x 1/CSF

Intake Factor Equation:
IF=BW x AT x 1/ED x 1/EF x 1/IR x 1/CF

Parameter Code	Parameter Definition	Units	Default Value	Rationale/ Reference	User Defined Value	Rationale/ Reference
CS	Target Soil Concentration	mg/kg	1.43E+00	calculated		
RL	Target Risk Level		1.00E-06	EPA		
CSF	Carcinogenic Slope Factor for PCBs	1/mg/kg-day	2.00E+00	EPA		
IR	Soil Ingestion Rate	mg/day	100	EPA		
EF	Exposure Frequency	days/year	250	EPA		
ED	Exposure Duration	years	25	EPA		
CF	Conversion Factor	kg/mg	1.E-06	EPA		
BW	Body Weight	kg	70	EPA		
AT	Averaging Time	days	25,550	EPA		
IF-C	Intake Factor (Cancer)	days	2.86E+06	calculated		

Appendix E.2

BSAF Based Target Sediment Concentrations

Chemical of Potential Concern	Target Sediment Concentration ug/kg	Target Sediment Concentration mg/kg	Target Tissue Concentration mg/kg	Biota-Sediment Concentration Factor (BSAF)	BSAF Reference	Location	Species	% Lipids	Sediment Organic Carbon
Total PCBs	1.80E+00	1.80E-03	5.39E-02	3.00E+01	EPA, 2001	Ontario Lake	Yellow Perch		
Total PCBs	2.01E+00	2.01E-03	5.39E-02	2.68E+01	EPA, 2001	Ontario Lake	Yellow Perch	2.55E-01	9.74E-02
Total PCBs	3.48E+00	3.48E-03	5.39E-02	1.55E+01	EPA, 2001	Ontario Lake	Smallmouth Bass		
Total PCBs	3.93E+00	3.93E-03	5.39E-02	1.37E+01	EPA, 2001	Ontario Lake	Yellow Perch	2.68E-01	5.29E-02
Total PCBs	4.24E+00	4.24E-03	5.39E-02	1.27E+01	EPA, 2001	Ontario Lake	Smallmouth Bass	1.22E+00	5.29E-02
Total PCBs	4.57E+00	4.57E-03	5.39E-02	1.18E+01	EPA, 2001	Ontario Lake	Yellow Perch	2.68E-01	7.64E-02
Total PCBs	4.90E+00	4.90E-03	5.39E-02	1.10E+01	Wong, 2001	Housatonic River, CT	White sucker	1.05E+01	1.30E+01
Total PCBs	5.04E+00	5.04E-03	5.39E-02	1.07E+01	EPA, 2001	Ontario Lake	Lake Trout	7.07E-01	5.29E-02
Total PCBs	7.38E+00	7.38E-03	5.39E-02	7.30E+00	EPA, 2001	Ontario Lake	Smallmouth Bass	5.32E-01	9.74E-02
Total PCBs	8.04E+00	8.04E-03	5.39E-02	6.70E+00	EPA, 2001	Ontario Lake	Smallmouth Bass	1.05E+00	7.64E-02
Total PCBs	8.16E+00	8.16E-03	5.39E-02	6.60E+00	EPA, 2001	Ontario Lake	Yellow Perch		
Total PCBs	8.55E+00	8.55E-03	5.39E-02	6.30E+00	Ashley, 2004	Delaware River	Channel Catfish		
Total PCBs	8.83E+00	8.83E-03	5.39E-02	6.10E+00	Ashley, 2004	Delaware River	White perch		
Total PCBs	8.98E+00	8.98E-03	5.39E-02	6.00E+00	EPA, 2001	Ontario Lake	Yellow Perch	1.50E-01	9.87E-02
Total PCBs	9.45E+00	9.45E-03	5.39E-02	5.70E+00	Wong, 2001	Quinebaug River, MA	White sucker	5.90E+00	7.80E+01
Total PCBs	9.45E+00	9.45E-03	5.39E-02	5.70E+00	Wong, 2001	Codorus Creek, PA	White sucker	6.00E+00	3.20E+01
Total PCBs	1.02E+01	1.02E-02	5.39E-02	5.30E+00	Ashley, 2004	Delaware River	Prey fish		
Total PCBs	1.06E+01	1.06E-02	5.39E-02	5.10E+00	EPA, 2001	Ontario Lake	Smallmouth Bass		
Total PCBs	1.22E+01	1.22E-02	5.39E-02	4.40E+00	Wong, 2001	Quinebaug River, CT	White sucker	6.70E+00	2.70E+01
Total PCBs	1.22E+01	1.22E-02	5.39E-02	4.40E+00	EPA, 2001	Ontario Lake	Yellow Perch		
Total PCBs	1.25E+01	1.25E-02	5.39E-02	4.30E+00	EPA, 2001	Ontario Lake	Lake Trout	5.65E+00	7.64E-02
Total PCBs	1.35E+01	1.35E-02	5.39E-02	4.00E+00	EPA, 2001	Ontario Lake	Smallmouth Bass	2.17E-01	9.87E-02
Total PCBs	1.42E+01	1.42E-02	5.39E-02	3.80E+00	EPA, 2001	Ontario Lake	Lake Trout	2.32E+00	9.87E-02
Total PCBs	1.42E+01	1.42E-02	5.39E-02	3.80E+00	EPA, 2001	Ontario Lake	Smallmouth Bass		
Total PCBs	1.63E+01	1.63E-02	5.39E-02	3.30E+00	Wong, 2001	EB Housatonic River, MA	White sucker	2.80E+00	2.20E+01
Total PCBs	1.86E+01	1.86E-02	5.39E-02	2.90E+00	Crimmins, 2002	Potomac River	Finfish		
Total PCBs	2.25E+01	2.25E-02	5.39E-02	2.40E+00	Wong, 2001	Quinnipiac River, CT	White sucker	5.90E+00	1.80E+01
Total PCBs	2.69E+01	2.69E-02	5.39E-02	2.00E+00	Wong, 2001	Mill River, MA	White sucker	3.60E+00	3.20E+01
Total PCBs	2.91E+01	2.91E-02	5.39E-02	1.85E+00	EPA, 2001		Salmonids		
Total PCBs	2.99E+01	2.99E-02	5.39E-02	1.80E+00	Wong, 2001	Mattabasset River, CT	White sucker	5.80E+00	3.20E+01
Total PCBs	2.99E+01	2.99E-02	5.39E-02	1.80E+00	Wong, 2001	French River, CT	White sucker	8.20E+00	3.70E+00
Total PCBs	4.90E+01	4.90E-02	5.39E-02	1.10E+00	Wong, 2001	Fanno Creek, OR	sculpins	5.00E+00	2.90E+01

Appendix E.2 Continued

VALUES USED FOR TARGET SEDIMENT CONCENTRATION CALCULATIONS

Medium:	Sediment
Exposure Medium:	Fish Tissue
Type	f
	F=Fish
	S=Shellfish
Exposure Route:	Ingestion
Receptor Age:	a
	A = Adult

Target Sediment Concentration:
CS=CT/BSAF

Target Tissue Concentration:
CT=RL x IF x 1/CSF

Intake Factor Equation:
IF=BW x PF x EDF x T x 1/MS x 1/NM

Parameter Code	Parameter Definition	Units	Default Value	Rationale/ Reference	User Defined Value	Rationale/ Reference
CS	Target Sediment Concentration	mg/kg	NA	calculated		
BSAF	Biota-Sediment Accumulation Factor	$(C_b/f_l)/(C_s/f_{oc})$	NA	literature values		
C_b	Concentration in Biota	ug/kg	NA	literature values		
f_l	biota lipid fraction	fraction by weight	NA	literature values		
C_s	Sediment Concentration	ug/kg	NA	literature values		
f_{oc}	Fraction organic carbon	fraction by weight	NA	literature values		
CT	Target Chemical Concentration in Tissue	mg/kg	5.39E-02	calculated		
RL	Target Risk Level		1.00E-05	VDH/DEQ		
CSF	Carcinogenic Slope Factor for PCBs	1/mg/kg-day	2.00E+00	EPA		
PF	Preparation Factor		2	VDH		
EDF	Exposure Duration Factor		2.33	VDH		
T	Time Period	days/month	30	VDH		
BW	Body Weight	kg	70	VDH		
MS	Averge Fish Meal Size	kg/meal	0.227	VDH		
NM	Number of Meals per month	meals/month	4	VDH		
IF-C	Intake Factor (Cancer)	days	1.08E+04	calculated		

Appendix E.3

BASS modeling of PCB bioaccumulation and Virginia watersheds

In short, the BASS modeling software uses sediment or water PCB concentrations to help predict what levels will end up in different species of fish. It considers modeling factors either variables or constants, for different habitats and other environmental conditions. A more detailed description and uses of BASS follow.

The BASS Bioaccumulation and Aquatic System Simulator has been under continuous development at the Ecosystems Research Division (ERD) of the USEPA National Exposure Research Laboratory (NERL) since the mid 1990s. Although originally developed to predict the bioaccumulation of organic industrial chemicals and pesticide in fish within a community/ecosystem framework, it has also been developed to simulate ecological exposures and responses of age-structured fish species and communities to organo-metallic compounds such as methyl mercury and to non-chemical stressors such as invasive/exotic species, fisheries management practices (stocking and harvesting), and various physical habitat alternations.

ERD researchers have used BASS to predict and analyze not only PCB bioaccumulation at the Twelve Mile Creek Superfund site at Lake Hartwell, SC but also methyl mercury bioaccumulation in the Florida Everglades. BASS has also been used to corroborate methyl mercury BAFs that were used in the USEPA Region IV mercury TMDL (Total Maximum Daily Loading). Most recently, BASS is being used to provide environmental analysts and other stakeholder groups in the Mid Atlantic Highlands a tool to investigate how fishery and watershed management practices would be expected to affect the ecological structure, function, and exposures of that region's streams.

A training course in the use and application of the BASS bioaccumulation and community model was held June 23-25, 2004 and attended by SWRO DEQ staff Nancy Norton and Craig Lott. The class size was small, however, this second introductory course to the use and application of the BASS model software and graphical users interface (GUI), dealt with some real world situations.

The course reviewed BASS's basic theoretical foundations, formulation, and chemical kinetics; however, the primary focus was the use and application of the BASS model software and GUI. The construction and development of previous and ongoing ERD applications of BASS were presented. The use of various BASS simulation options were reviewed and demonstrated. The structure and function of BASS's file/project management system were reviewed and discussed in terms of how to create new BASS applications by the selective addition or editing of existing project 'include' files.

Although many differences exist between those in-class examples and Virginia's watersheds, the organization of the model in breaking down the contributions and relationships between different variables was extremely useful and allows the relationships to be quantified. Existing detailed Virginia watershed and species data is available and variables or constants can be determined. The usefulness of the model lies is in its flexibility. Work requiring a general accuracy allows for simplification of the model and use of constants for certain relationships and variables. If a project requires a greater accuracy, the effects of more complex relationships can be included, such as habitat; water temperature; plant and animal food chain levels, food availability, and species related factors; congener vs. total PCB definitions and partitioning coefficients, bioaccumulation and toxicity differences; PCB oil exposure routes and time variance; mobility of target species and individuals; weather; seasons, etc.

Additionally, the new GUI, graphical user interface, is very user-friendly and requires little training. The output graphs are extremely helpful to understand the relationships between different contamination scenarios and the real life potential. In other words risk assessment for long term exposure periods versus cleanup can be examined. Once a watershed is modeled, the differences of potential exposure routes can be examined to help define the existing fish and sediment PCB or other Persistent Bioaccumulative Toxin, PBT, results.

Contact info for Questions regarding this training course or the BASS software itself are below:

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Several problems within our state appear to be covered by this type model. Once the model is setup for any specific waterbody/fish/habitat scenario, most data and relationships would not vary, and then given different contamination events, potential exposure and bioaccumulation could be determined.

Uses of the BASS model include

1. Estimation of spill effects of PCBs, methyl mercury, other industrial organic pollutants, or other Persistent Bioaccumulative Toxins, PBTs;
2. Estimation or measurement of the potential long-term contamination problems (fishable use or swimable use criteria);
3. TMDL support;
4. Risk Assessment; and
5. Potentially to back calculate/estimate using the iterative process and known fish tissue concentrations, what the soil or sediment contamination levels or to stretch the process even further with enough biological data, perhaps the extent of or locations of unknown PCB point sources.

One of my goals for attending the training was to use the BASS model to help back calculate a level of PCBs in sediment that would just reach the 54 ppb fish tissue concentration advisory level. It turns out that this can be done with a fairly simple model developed from the BASS model, but it uses many assumptions and simplifications of relationships to determine a number which approximates some of our state water-fish-contaminant systems. Craig Barber and I developed a 'PCBs in Virginia fish from sediment concentrations draft calculation' over the phone and emails. Later I put this calculation into a spreadsheet format for ease of use. The development of the calculations follows this paragraph and the spreadsheet is attached as an MS Excel file 'Sed-PCB calc from Fish-PCB.xls' :

The equilibrium thermodynamic relationship between PCB sediment and water concentrations is given by

$$\frac{[PCB\,]_{sediment}}{[PCB\,]_{water}} = f_{oc}\ K_{oc}$$

(1)

$$[PCB\,]_{water} = \frac{[PCB\,]_{sediment}}{f_{oc}\ K_{oc}}$$

where $K_{oc} = 0.4\ K_{ow}$.

Similarly, the equilibrium thermodynamic relationship between PCB fish and water concentrations is given by

$$\frac{[PCB\,]_{fish}}{[PCB\,]_{water}} = BAF$$

(2)

$$[PCB\,]_{fish} = [PCB\,]_{water}\ \ BAF$$

When Equations (1) and (2) are combined, it then follows that at equilibrium that

$$[PCB\,]_{fish} = \frac{BAF\quad [PCB\,]_{sediment}}{f_{oc}\;0.4\;\;K_{ow}} \quad \textbf{(3)}$$

If the fishery advisory threshold is set at 54 ppb, it also follows that

$$54 \;>\; [PCB\,]_{fish}$$

$$54 \;>\; \frac{BAF\quad [PCB\,]_{sediment}}{f_{oc}\;0.4\;\;K_{ow}} \qquad \textbf{(4)}$$

$$\frac{54\quad f_{oc}\;0.4\;\;K_{ow}}{BAF} \;>\; [PCB\,]_{sediment}$$

where fish and sediment concentrations are in units of ppb = ng (PCB) / g (wet weight).

To parameterize Expression (4) for total PCBs, the K_{ow} can be estimated as the mean of log K_{ow} for tetra-, penta-, hexa-, and hepta-PCBs. Thus,

$$\log\;K_{ow} = \frac{5.91+6.34+6.75+7.19}{4}$$

$$K_{ow} = 10^{6.55} \qquad \textbf{(5)}$$

Substituting this equation into Expression (4) then yields

$$\frac{21.6\;\;10^{6.55}\;\;f_{oc}}{BAF} \;>\; [PCB\,]_{sediment} \quad \textbf{(6)}$$

Model predicted log BAF? s for tetra-, penta-, hexa-, and hepta-PCBs in catfish, sunfish, and largemouth bass typically range from 4.91 to 5.94 with a mean equal to 5.27. When this mean is substituted into Expression (6), one how obtains

$$\frac{21.6\;\;10^{6.55}\;\;f_{oc}}{10^{5.27}} \;>\; [PCB\,]_{sediment}$$

$$f_{oc}\;10^{2.61} \;>\; [PCB\,]_{sediment} \qquad \textbf{(7)}$$

Finally assuming a nominal 2.5% organic carbon content for PCB-contaminated sediments one would expect fish to be under the 54 ppb action only when

$$10.2 > [PCB]_{sediment} \quad \textbf{(8)}$$

Assuming a nominal sediment conversion ratio of 1.46 g (wet)/g (dry) for sediment porosities varying from 0.5-0.6, the preceding expression is also equivalent to

$$14.9 > [PCB]_{sediment,dry} \quad \textbf{(9)}$$

Note, however, there are many uncertainties regarding the above screening calculation; These include

- ? equilibrium between sediment and water column PCB concentrations
- ? time varying vs. constant exposures
- ? treating PCBs and a single chemical (e.g., not addressing differences in congener K_{ow})
- ? the ecology and physiology of the target fish species (i.e., growth rates, dietary composition, lipid contents, mobility, etc.)

Appendix E.4

BASS Model Screening Calculations

		Value	Units
INPUT:	Virginia's PCB in edible fish tissue fillets consumption advisory level	54	ppb
	organic fraction of sediment	2.50%	percent
	Percent Moisture of Sediment	30.00%	percent
	If interested, input here various PCB concentrations in fish tissues		ppb

Problem:	**What wet Sediment PCB concentration causes fish to be greater than the known fish tissue concentrations?**	**10.29**	**ppb**
	What dry Sediment PCB concentration causes fish to be greater than the known fish tissue concentrations?	**14.70**	**ppb**
	dry Sediment PCB concentration using 1.46 as the 'pore-size moisture' factor	**15.02**	**ppb**

PCB concentration in fish tissues used in calculations 54.00 ppb

Solution: We want fish < 54 ppb or < 0.054 ppm

Since the equilibrium thermodynamic relationship can be represented by the following equation

$[PCB]_{sediment} / [PCB]_{water} = f_{OC} * K_{OC}$

then by rearrangement, $[PCB]_{sediment} = f_{OC} * K_{OC} * [PCB]_{water}$

where f_{OC} is organic carbon fraction of sediment

and where K_{OC} is the sediment partitioning coefficient for PCB oils.

Also since for most conditions … $K_{OC} = 0.4\ K_{OW}$

where K_{OW} is the water partitioning coefficient for PCB oils.

then by substitution, $[PCB]_{sediment} = f_{OC} * (0.4 * K_{OW}) * [PCB]_{water}$

Also since, Bioaccumulation Factor = $BAF = [PCB]_{fish} / [PCB]_{water}$

next by rearrangement, $[PCB]_{water} = [PCB]_{fish} / BAF$

and then by substitution, $[PCB]_{sediment} = f_{OC} * (0.4 * K_{OW}) * [PCB]_{fish} / BAF$

Since the state of Virginia VDH and VaDEQ use total PCBs to help define toxicity and advisory levels, we will estimate an expression using some of the bioaccumulative toxic PCB congeners' known partitioning coefficients for tetra-, penta-, hexa-, and hepta-PCBs…

$\log K_{OW} = (5.91 + 6.34 + 6.75 + 7.19) / 4 = 6.55$

$K_{OW} = 10^{6.55}$

Also, since BASS model predicted "log BAF's" for tetra-, penta-, hexa-, and hepta-PCBs in catfish, sunfish, and largemouth bass typically range from 4.91 to 5.94 we can determine a mean log BAF equal to 5.27.

Upon substitution of these values, $[PCB]_{sediment} = f_{OC} * (0.4 * K_{OW}) * [PCB]_{fish} / BAF$

or, $\mathbf{[PCB]_{sediment} = f_{OC} * (0.4 * 10^{6.55}) * [PCB]_{fish} / 5.27}$

NOTE: Regarding uncertainties in the above screening equation, these include the following...

1. equilibrium between sediment and water column PCB concentrations vary with water and sediment quality and environmental conditions.
2. time varying versus constant exposures of fish to PCBs.
3. treating PCBs as a single chemical (i.e., 'total PCBs'; not addressing the actual differences in congener KOW)
4. the ecological and physiological aspects of the target fish species have been ignored or assumed to be negligible, but could vary greatly in real world dynamics (i.e., growth rates, dietary composition, lipid contents, mobility of species, ambient water temp, etc.).

Appendix E.5

Percentile Values for DEQ PCB Data Sets

Table 1. Combined data (VIMS) from the statewide Fish Tissue & Sediment Monitoring Program plus special studies on the New and James Rivers (excluding non-detects and 0.0s).

Total PCB Conc. ng/g	Percentile	Summary Statistics	value
7,668.2	99th	Count (n)	667
746.6	95th	Minimum (ng/g)	0.07
99.9	90th	Maximum (ng/g)	82,235
49.2	85th	Average (ng/g)	395.3
27.2	80th		
17.9	75th		
4.2	50th		
1.3	25th		

Table 2. VIMS data generated for the statewide Fish Tissue & Sediment Monitoring Program (excluding non-detects and 0.0s).

Total PCB Conc. ng/g	Percentile	Summary Statistics	value
1,847.2	99th	Count (n)	583
104.7	95th	Minimum (ng/g)	0.07
49.4	90th	Maximum (ng/g)	82,235
26.3	85th	Average (ng/g)	197.71
17.2	80th		
12.6	75th		
3.3	50th		
1.1	25th		

Table 3. VIMS data generated for PRO's James River special studies (1997-1998 & 2003).

Total PCB Conc. ng/g	Percentile	Summary Statistics	value
15,383	99th	Count (n)	51
4,444.5	95th	Minimum (ng/g)	0.1
1,995	90th	Maximum (ng/g)	24,979
1,856.5	85th	Average (ng/g)	1,086.1
775.5	80th		
463.7	75th		
35.8	50th		
9.3	25th		

Table 4. VIMS data generated for WCRO's New River PCB special study.

Total PCB Conc. ng/g	Percentile	Summary Statistics	value
27,915.4	99^{th}	Count (n)	32
13,593.4	95^{th}	Minimum (ng/g)	1.78
7,945.3	90^{th}	Maximum (ng/g)	32,558
7,669.1	85^{th}	Average (ng/g)	2,907
2,763	80^{th}		
1,322.3	75^{th}		
79.2	50^{th}		
9.8	25^{th}		